

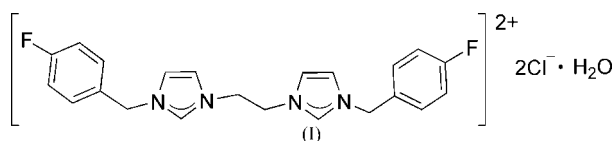
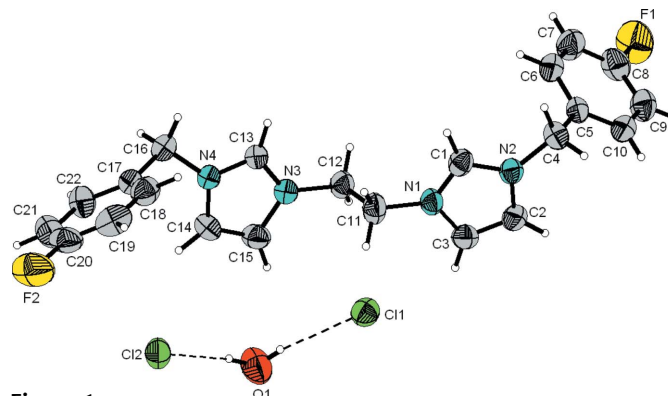
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## Key indicators

Single-crystal X-ray study  
 $T = 273$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.043  
 $wR$  factor = 0.124  
Data-to-parameter ratio = 17.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.1,1'-Bis(4-fluorobenzyl)-3,3'-ethylene-  
diimidazolium dichloride monohydrateIn the title compound,  $\text{C}_{22}\text{H}_{22}\text{F}_2\text{N}_4^{2+} \cdot 2\text{Cl}^- \cdot \text{H}_2\text{O}$ , the two imidazole rings are in a *syn* orientation with respect to each other. The crystal structure displays  $\text{O}-\text{H} \cdots \text{Cl}$ ,  $\text{C}-\text{H} \cdots \text{Cl}$ ,  $\text{C}-\text{H} \cdots \text{F}$  and  $\text{C}-\text{H} \cdots \text{O}$  hydrogen bonds.Received 7 December 2006  
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## Comment

Our group is interested in the preparation of imidazolium salts, which can be employed as ligand precursors for *N*-heterocyclic carbenes. In our previous work (Lee *et al.*, 2004), we reported the preparation of 1,1'-di(4-fluorobenzyl)-3,3'-ethylenediimidazolium dichloride and its palladium(II) complex. We report here the crystal structure of the title compound, (I) (Fig. 1). The structures of the related 1,1'-bis(1-naphthalenemethyl)-3,3'-ethylenediimidazolium dichloride, (II), and 1,1'-dibenzyl-3,3'-ethylenediimidazolium dichloride, (III), have also been reported by us (Lee *et al.*, 2004).The asymmetric unit of (I) contains a  $\text{C}_{22}\text{H}_{22}\text{F}_2\text{N}_4^{2+}$  dication, two chloride anions and a water molecule. The water molecule presumably came from the wet solvent used in crystallization. Interestingly, the water molecule forms two hydrogen bonds with the chloride anions (Table 1). The two imidazole rings are in a *syn* orientation with respect to each other. Similar hydrogen-bonding interactions and *syn* orientation were found in the structure of (II) (Lee *et al.*, 2004). In contrast, in the structure of (III), which contains no guest

**Figure 1**  
The molecular structure of (I), showing 50% probability displacement ellipsoids for non-H atoms. Hydrogen bonds are shown as dashed lines.

water molecule, the two imidazole rings are in *trans* orientation (Lee *et al.*, 2004).

The crystal packing is also stabilized by C—H···Cl, C—H···F and C—H···O hydrogen bonds (Table 1).

### Experimental

The title compound was prepared according to a literature procedure (Lee *et al.*, 2004). Single crystals were obtained by slow diffusion of diethyl ether into a dimethylformamide solution of (I) at room temperature.

#### Crystal data

$C_{22}H_{22}F_2N_4^{2+} \cdot 2Cl^- \cdot H_2O$	$V = 1140.5 (2) \text{ \AA}^3$
$M_r = 469.35$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.367 \text{ Mg m}^{-3}$
$a = 8.6232 (11) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 10.7019 (13) \text{ \AA}$	$\mu = 0.32 \text{ mm}^{-1}$
$c = 12.7024 (16) \text{ \AA}$	$T = 273 (2) \text{ K}$
$\alpha = 78.409 (4)^\circ$	Plate, colorless
$\beta = 84.100 (4)^\circ$	$0.23 \times 0.21 \times 0.10 \text{ mm}$
$\gamma = 85.743 (4)^\circ$	

#### Data collection

Bruker SMART APEX II diffractometer	9371 measured reflections
$\omega$ scans	4918 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	2819 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.911$ , $T_{\max} = 0.969$	$R_{\text{int}} = 0.033$
	$\theta_{\max} = 27.0^\circ$

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0544P)^2 + 0.0086P]$
$R[F^2 > 2\sigma(F^2)] = 0.043$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.124$	$(\Delta/\sigma)_{\max} = 0.001$
$S = 0.96$	$\Delta\rho_{\max} = 0.20 \text{ e \AA}^{-3}$
4918 reflections	$\Delta\rho_{\min} = -0.21 \text{ e \AA}^{-3}$
288 parameters	
H atoms treated by a mixture of independent and constrained refinement	

**Table 1**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1—H1···Cl1	0.77 (4)	2.40 (4)	3.158 (3)	168 (4)
O1—H2···Cl2	0.90 (4)	2.18 (4)	3.074 (3)	172 (3)
C1—H1A···Cl1 <sup>i</sup>	0.93	2.73	3.553 (3)	148
C2—H2A···F2 <sup>ii</sup>	0.93	2.54	3.242 (3)	133
C4—H4B···Cl1 <sup>i</sup>	0.97	2.82	3.702 (2)	151
C9—H9A···Cl2 <sup>iii</sup>	0.93	2.74	3.629 (3)	162
C13—H13A···O1 <sup>i</sup>	0.93	2.57	3.265 (4)	132
C16—H16A···Cl1 <sup>iv</sup>	0.97	2.64	3.600 (2)	169
C16—H16B···Cl2 <sup>i</sup>	0.97	2.82	3.687 (3)	150

Symmetry codes: (i)  $x-1, y, z$ ; (ii)  $x, y-1, z+1$ ; (iii)  $x-1, y-1, z+1$ ; (iv)  $-x+1, -y+1, -z+1$ .

Atoms H1 and H2 were located in a difference map and refined isotropically. The remaining H atoms were positioned geometrically (C—H = 0.93 or 0.97  $\text{\AA}$ ) and refined in the riding-model approximation, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 1998); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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### References

- Bruker (2004). APEX2 (Version 1.0-22) and SAINT (Version 6.280a). Bruker AXS Inc., Madison, Wisconsin, USA.
- Lee, H. M., Lu, C. Y., Chen, C. Y., Chen, W. L., Lin, H. C., Chiu, P. L. & Cheng, P. Y. (2004). *Tetrahedron*, **60**, 5807–5825.
- Sheldrick, G. M. (1998). SHELXTL. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (2003). SADABS. Version 2.10. University of Göttingen, Germany.